Numerical Techniques for Correction of Biases In Greenhouse Gas Fluxes Determined Using Non-Steady State Chamber Methods

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Agricultural Research Service

-USDA-NIFA Air Quality Program
-ARS GRACEnet Project

ASA-CSSA-SSSA Annual Meeting
18 October 2011, San Antonio

Non-steady state (NSS) Chamber Methods

Most commonly used method for measuring soil-to-atmosphere fluxes of GHGs (e.g. N_2O).

Open-bottomed chamber placed on soil surface, followed by sampling of chamber headspace at discrete time intervals; flux is determined from rate of increase in gas concentration.

Many advantages: Inexpensive, easy to implement, well-suited to replicated plot studies comparing treatment effects.

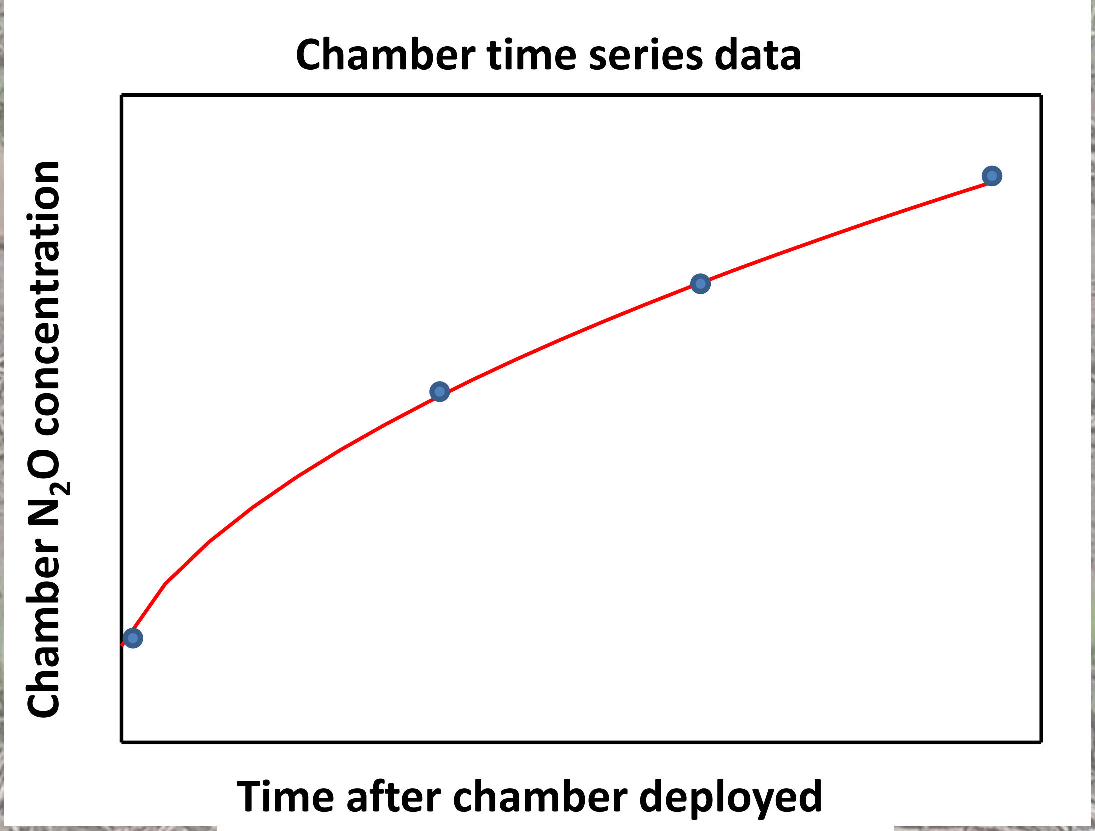
Important limitation: Chamber placement alters the flux, by disrupting the concentration gradient.

The “Chamber Effect”

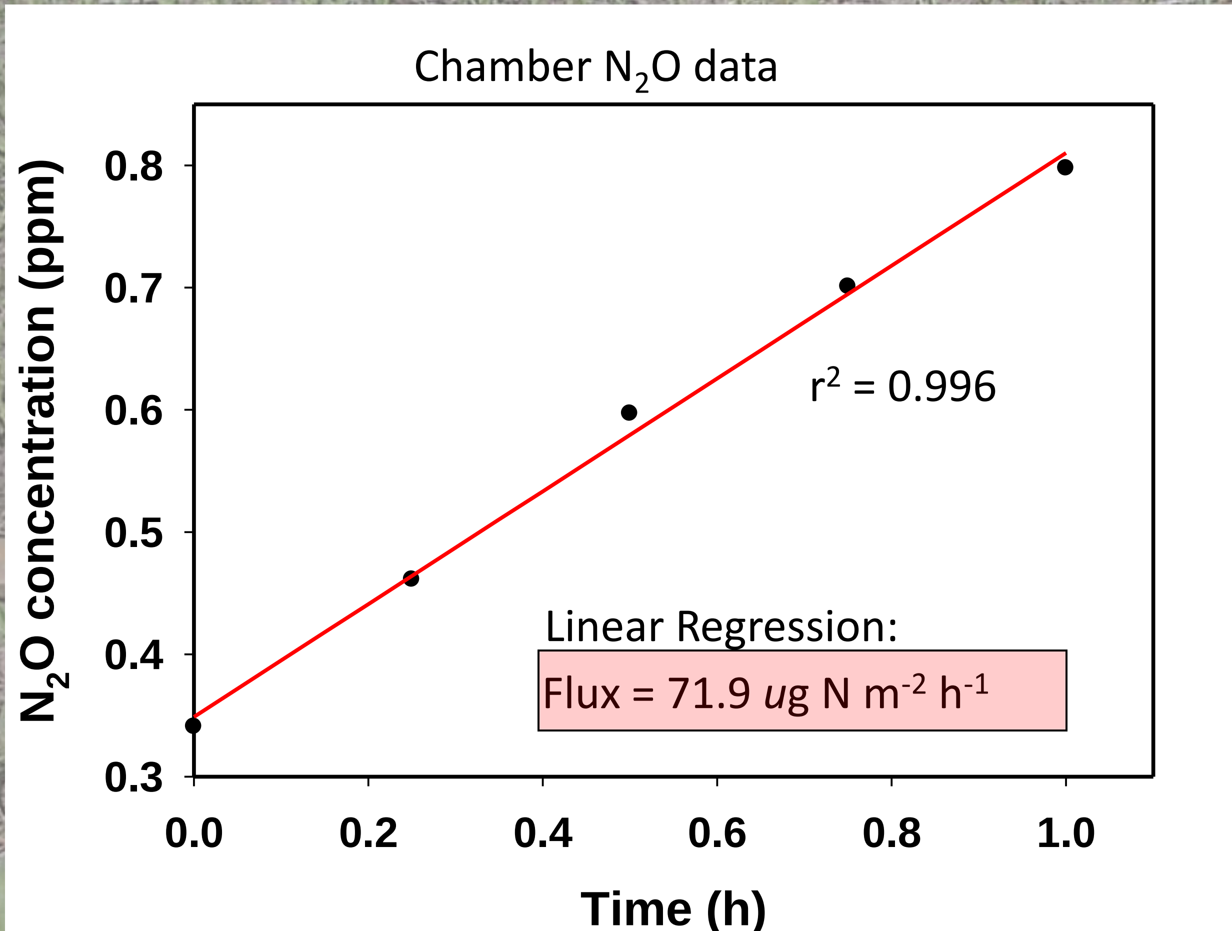
- Accumulation of gas suppresses diffusion, leads to non-linearity in chamber data (slope decreases with time)

- Flux at time zero will be underestimated using Linear Regression (LR)

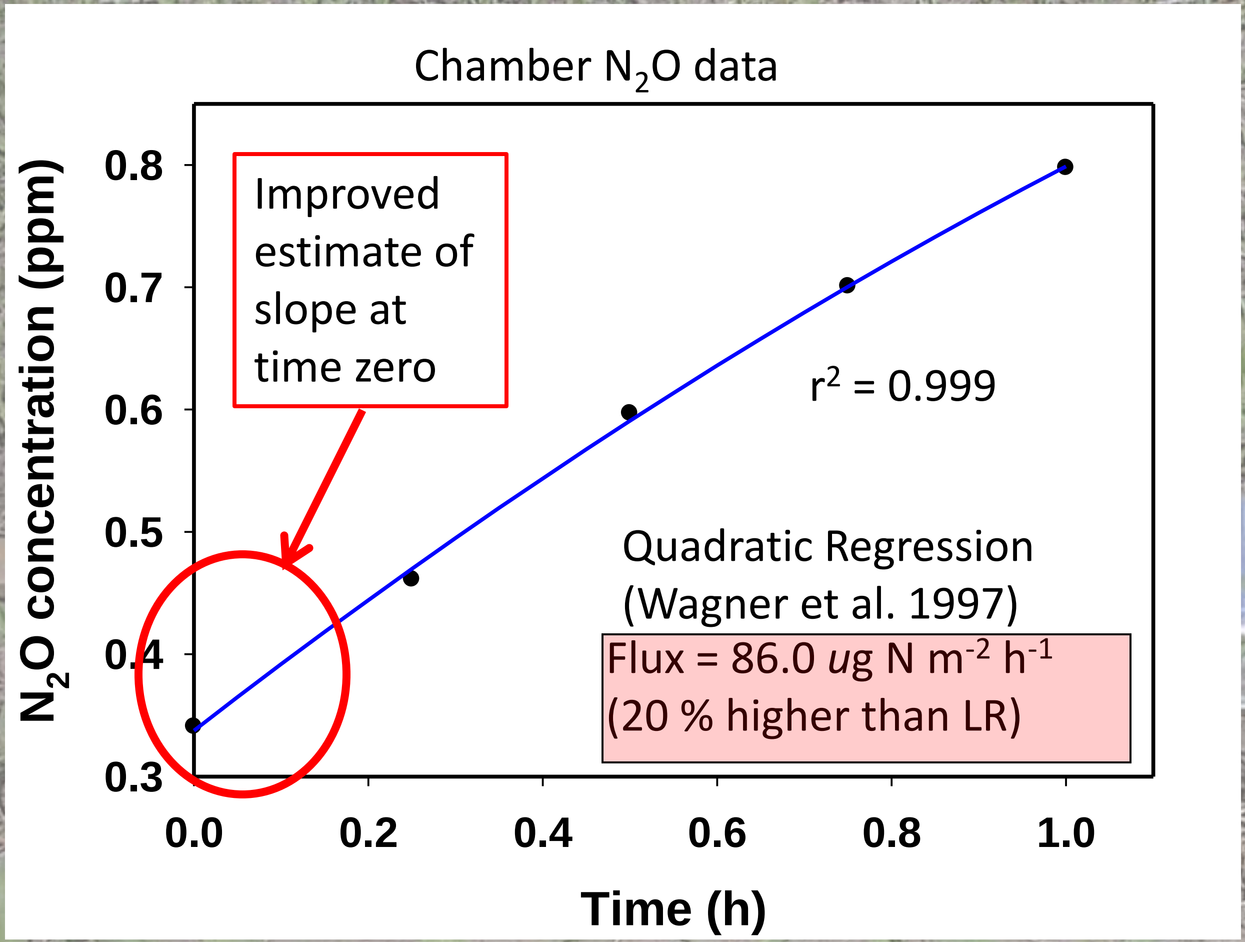
- Non-linear models have been developed to overcome this problem



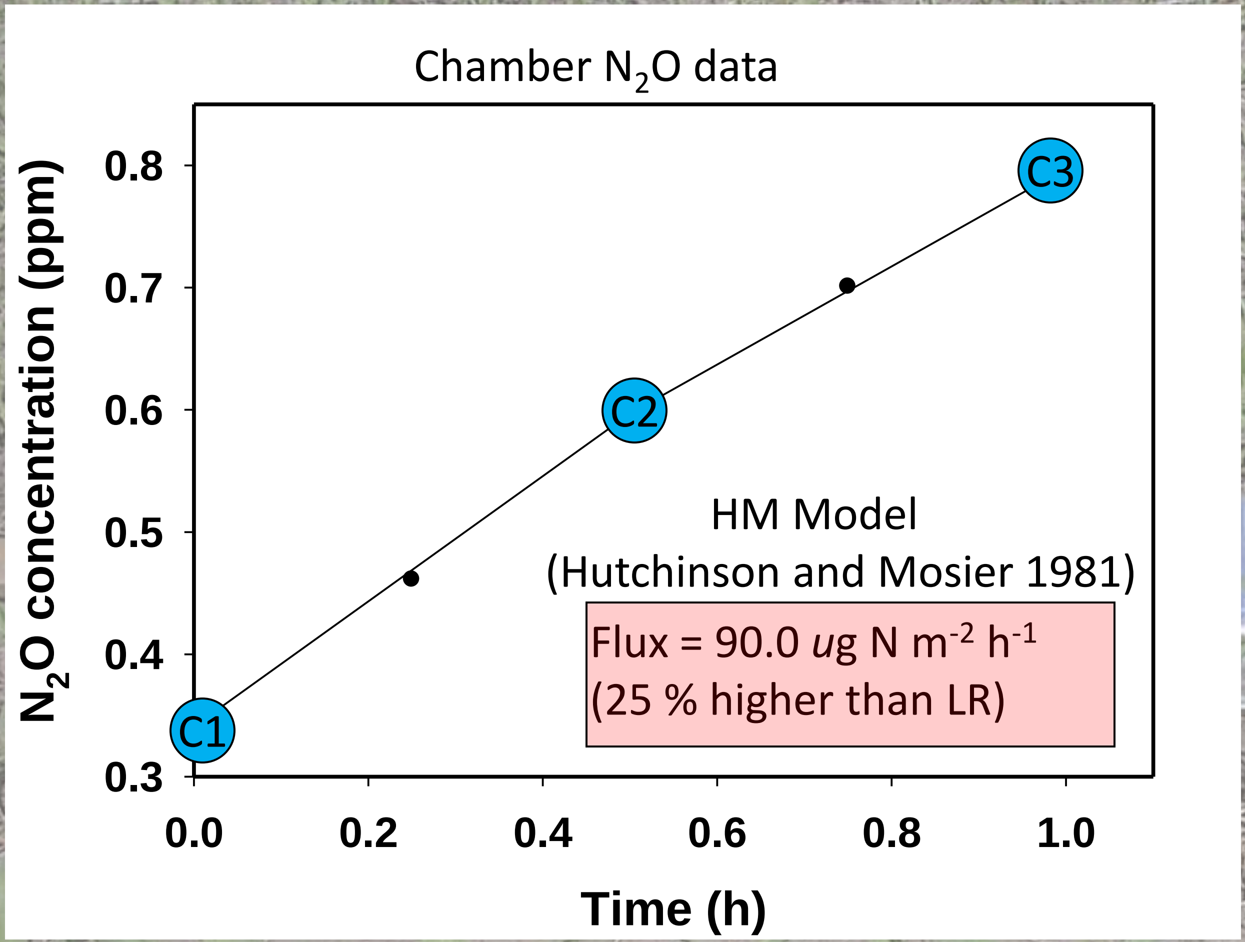
The “Chamber Effect” (example)



The "Chamber Effect" (example)

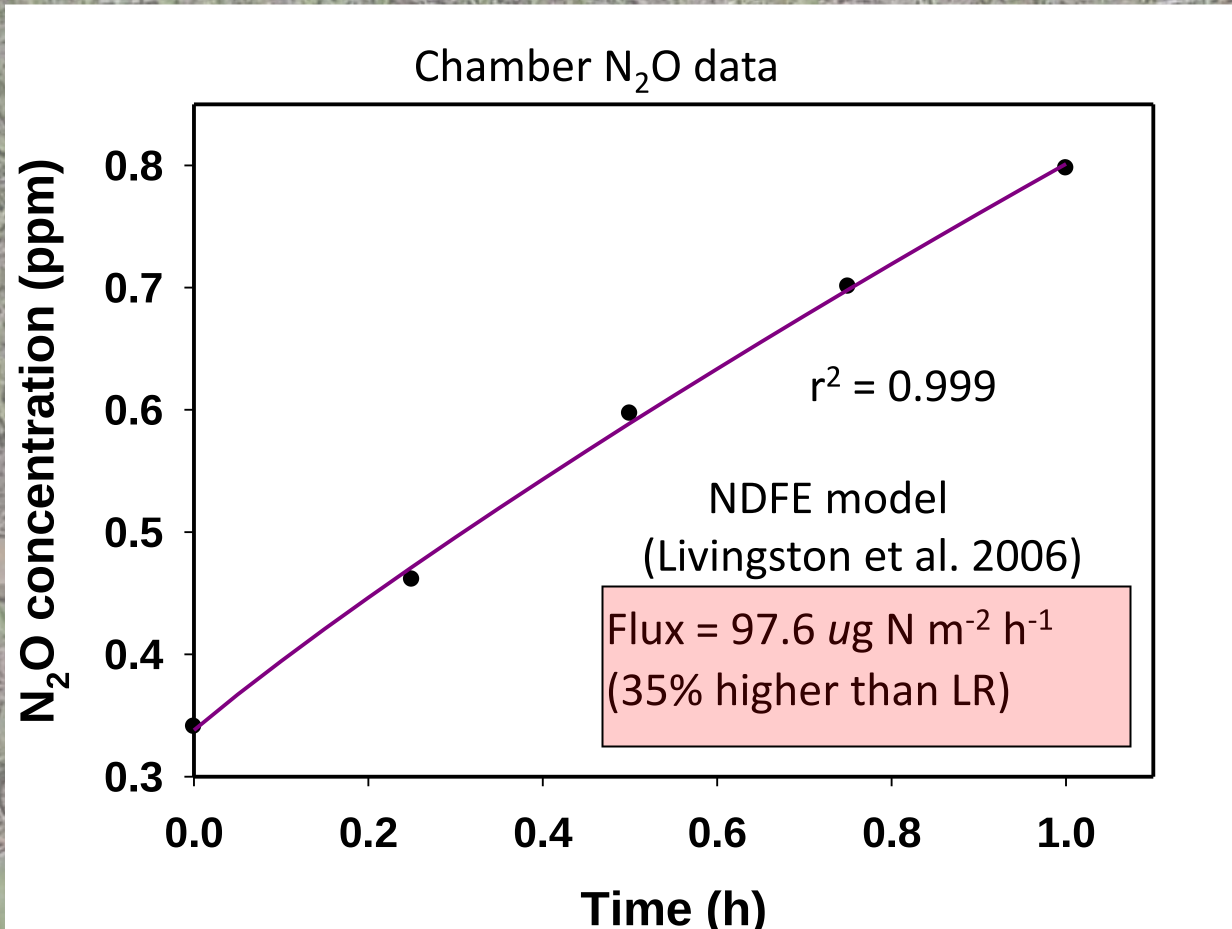


The “Chamber Effect” (example)



Problem solved?

The “Chamber Effect” (example)



Problem solved?

No !

Livingston et al. (2006)

• Even the HM and Quadratic Regression models can substantially under-estimate the pre-deployment flux.

• The extent of underestimation will increase with:

1. Smaller chamber volume to area ratio (i.e., shorter chamber height)
2. Longer chamber deployment times
3. Greater soil air-filled porosity

↓

Increased non-linearity in chamber data

↓

Increased negative bias of the flux estimate

↓

Errors of up to 40%

Failure of HM and Quadratic models

1. Quadratic regression: Fully empirical polynomial fit to data

$$C(t) = at^2 + bt + c$$

$$Flux_0 = H\,b, \text{ where H is height of chamber}$$

2. HM model: Theoretical basis, but very simplified

Governing equation is simple ODE: $\frac{dC}{dt} = k(C_d - C)$, where $k = \frac{D_s}{Hd}$

Simplifying assumptions:

$$Flux_0 = H D_s \frac{(C_d - C_0)}{d}$$

-Constant soil-gas concentration (C_d) is maintained at some depth *d*

-No gas is produced in soil above the depth *d*

-Flux is described by steady-state diffusion (linear concentration profiles)

Does not rigorously describe soil-gas diffusion

Livingston et al. (2006)

3. Non-steady-state Diffusive Flux Estimator (NDFE) Model: More rigorous theoretical basis

More realistic governing equation (PDE):

$$S\frac{\partial C}{\partial t} = D_s\frac{\partial^2 C}{\partial z^2} + P(z)$$

Accounts for:

-**Transient change in soil-gas storage *(1st term)***

-**Non-steady state gas diffusion in the soil profile *(2nd term)***

-**Arbitrary vertical distribution of the source term for N_2O production *(3rd term)***

Derived analytical solution for the PDE with BC accounting for accumulation of gas within a chamber of height H:

$$C_t = C_0 + Flux_0\frac{\tau}{H}\left[\frac{2}{\sqrt{\pi}}\sqrt{t/\tau} + \exp(t/\tau)erfc(\sqrt{t/\tau}) - 1\right]$$

The NDFE flux-calculation model
Livingston et al. (2006)

Implicit solution for *Flux₀*

$$C_t = C_0 + Flux_0 \frac{\tau}{H}\left[\frac{2}{\sqrt{\pi}}\sqrt{t/\tau} + \exp(t/\tau)erfc(\sqrt{t/\tau}) - 1\right]$$

-Developed non-linear regression code to solve for $Flux_0$

-Practical limitations: converges to multiple solutions, requires at least 4 and preferably 5 time points, not easily adapted to spreadsheet calculations.

-Not widely used.

However:

1. **Underlying theory is robust**
2. **Analytical solution can be useful in other ways**

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Usefulness of Analytical Solution
Livingston et al. (2006)

$$C_t = C_0 + Flux_0 \frac{\tau}{H}\left[\frac{2}{\sqrt{\pi}}\sqrt{t/\tau} + \exp(t/\tau)erfc(\sqrt{t/\tau}) - 1\right]$$

1. Allows for error analysis

Soil properties, chamber conditions, and an initial flux magnitude are assumed → A.S. used to generate chamber time series data for given set of conditions → Flux is calculated using available models (HM, Quad) → Calculated flux is compared with flux used in model input to determine error (bias)

Venterea (2010)

Usefulness of Analytical Solution
Livingston et al. (2006)

$$C_t = C_0 + Flux_0 \frac{\tau}{H}\left[\frac{2}{\sqrt{\pi}}\sqrt{t/\tau} + \exp(t/\tau)erfc(\sqrt{t/\tau}) - 1\right]$$

2. When the bias is expressed relative to the actual *Flux₀*:

$$\%\ flux\ underestimation = 100 * \frac{(Flux_0 - Estimated\ flux)}{Flux_0}$$

it is independent of the flux magnitude or source vertical distribution, so results can be more broadly generalized

Venterea (2010)

Usefulness of Analytical Solution
Livingston et al. (2006)

$$C_t = C_0 + Flux_0 \frac{\tau}{H}\left[\frac{2}{\sqrt{\pi}}\sqrt{t/\tau} + \exp(t/\tau)erfc(\sqrt{t/\tau}) - 1\right]$$

3. Tau term has physical meaning

$$\tau = \frac{H^2}{S\ D_s}$$

H = chamber height (volume to area ratio)
S = Soil-gas storage term
D_s = Soil diffusion coefficient

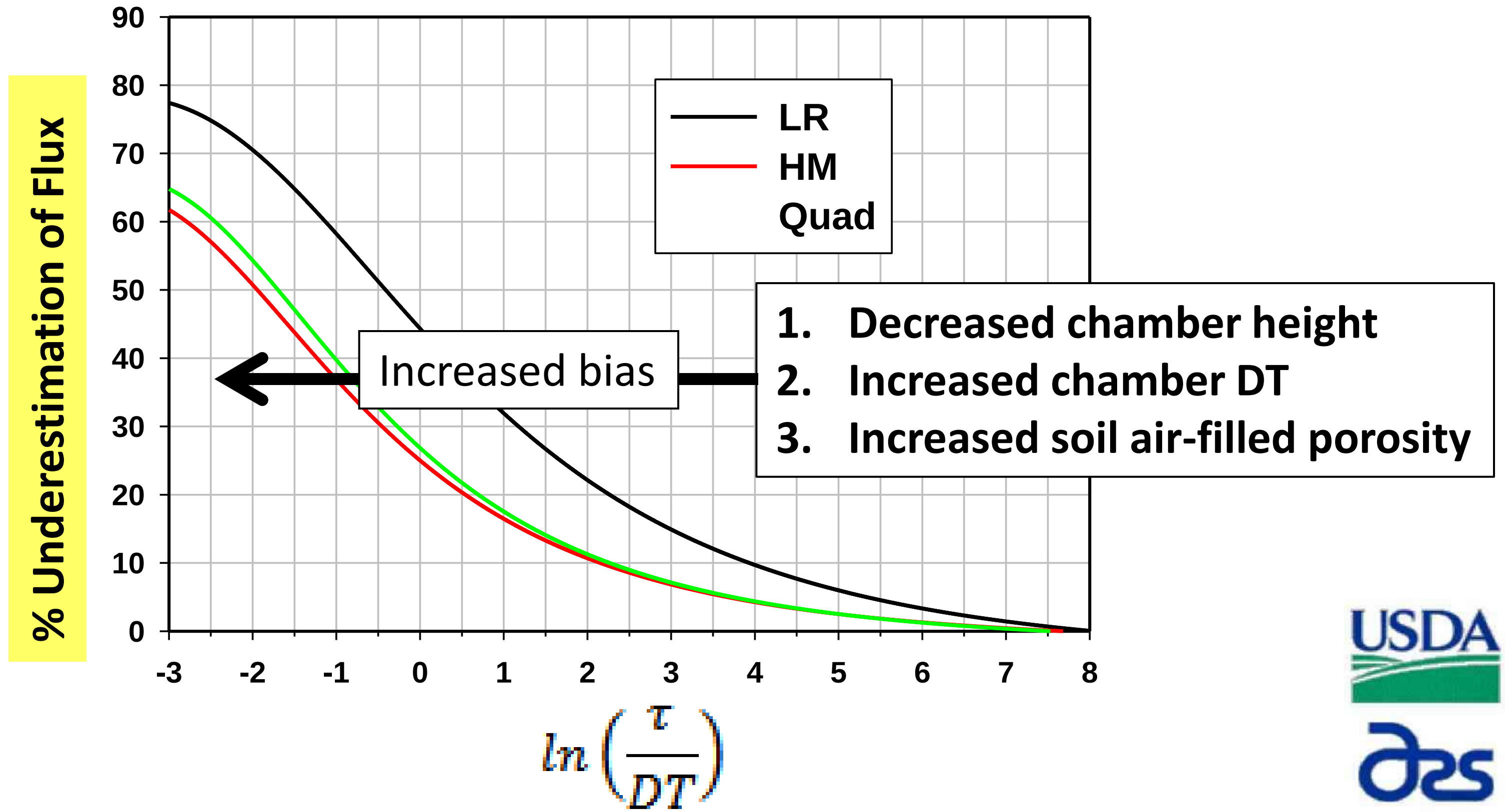
S and D_s can be further defined as functions of:
bulk density, porosity, water content, Henry's law constant, and temperature - all of which can be measured or estimated

Venterea (2010)

Usefulness of Analytical Solution
Livingston et al. (2006)

$$C_t = C_0 + Flux_0 \frac{\tau}{H}\left[\frac{2}{\sqrt{\pi}}\sqrt{t/\tau} + \exp(t/\tau)\,erfc(\sqrt{t/\tau}) - 1\right]$$

4. Bias for a given flux-calculation model can be expressed as empirical functions of τ and the chamber deployment time (DT):



Venterea (2010)

Error Sensitivity Analysis

Chamber height

Deployment time

Soil properties

Flux calculation method

Using hypothetical values

Flux-Estimation Error Analysis

Range of variation in flux-measurement bias:

Used in initial stages of designing chamber protocols.

Error Sensitivity Analysis

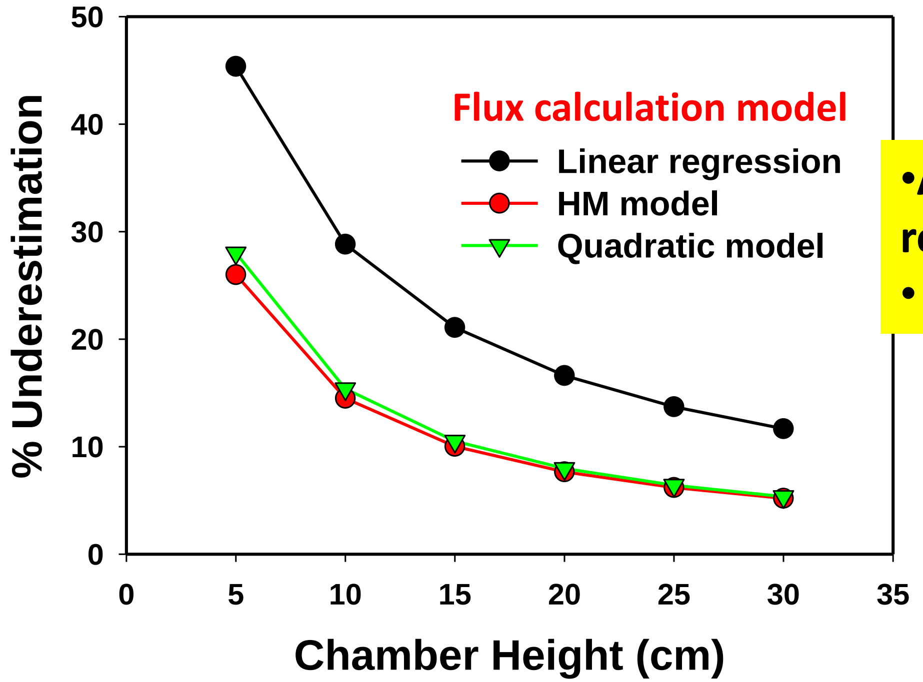
Chamber height
Variable (5 – 30 cm)

Deployment time
= 40 min

Soil properties
Bulk density = 1.1 g cm^{-3}
Water content = 0.15 g g^{-1}

Flux calculation method
Compare LR, Quadratic, HM

Flux-Estimation Error Analysis



- Approx. ½ of bias removed with NL models
- HM and Quad agree well

Venterea et al. (2009)

Error Sensitivity Analysis

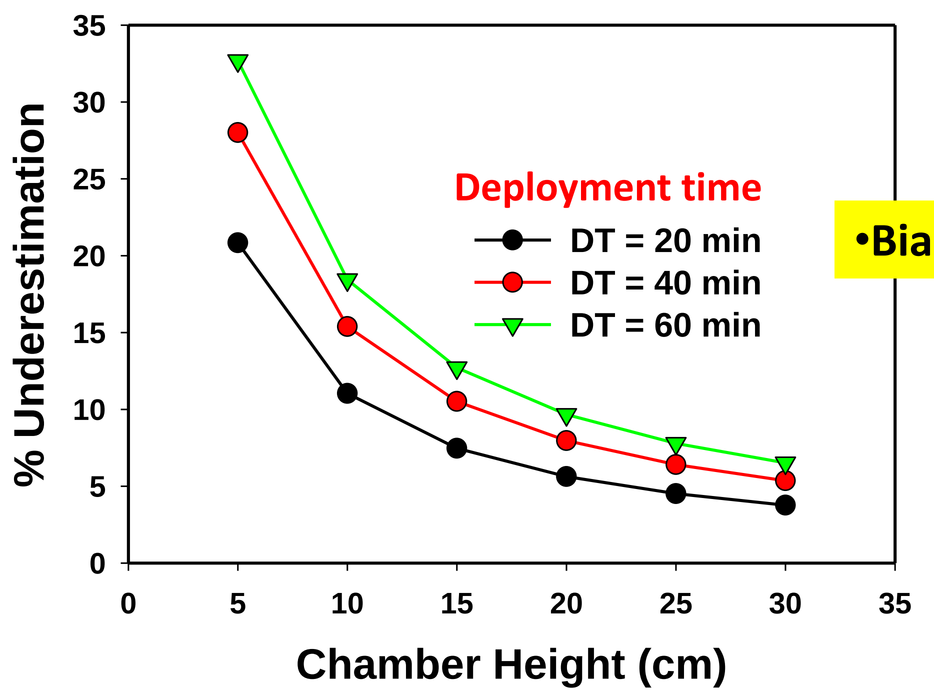
Chamber height
Variable (5 – 30 cm)

Deployment time
Compare 20, 40, 60 min

Soil properties
Bulk density = 1.1 g cm^{-3}
Water content = 0.15 g g^{-1}

Flux calculation method
Quadratic

Flux-Estimation Error Analysis



•Bias highly sensitive to DT

Venterea et al. (2009)

Error Sensitivity Analysis

Chamber height
Variable (5 – 30 cm)

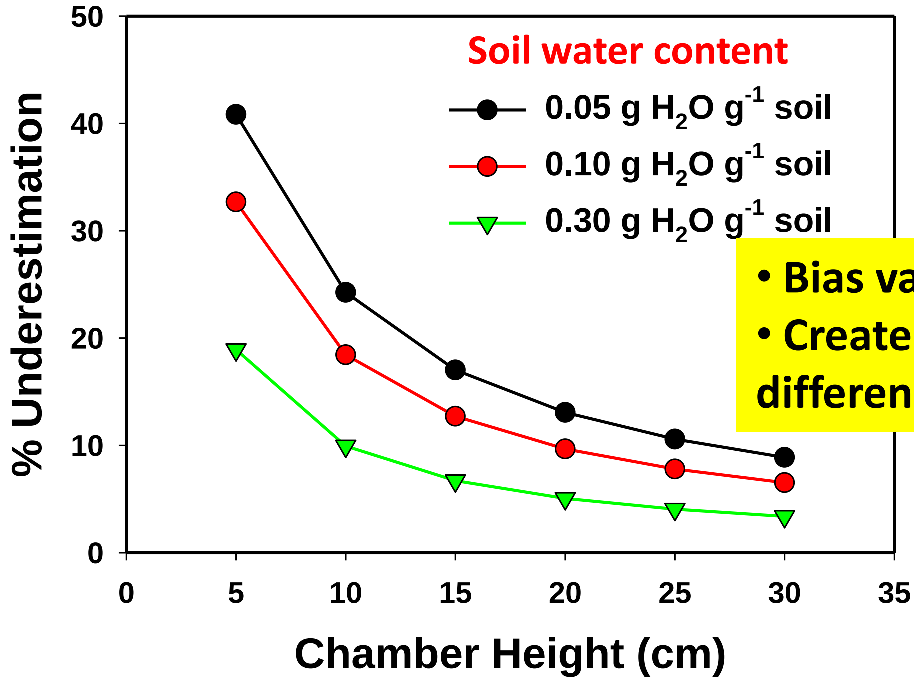
Deployment time
40 min

Soil properties
Bulk density = 1.1 g cm^{-3}

Compare water contents of 0.05, 0.10, and 0.30 g g^{-1}

Flux calculation method
Quadratic

Flux-Estimation Error Analysis

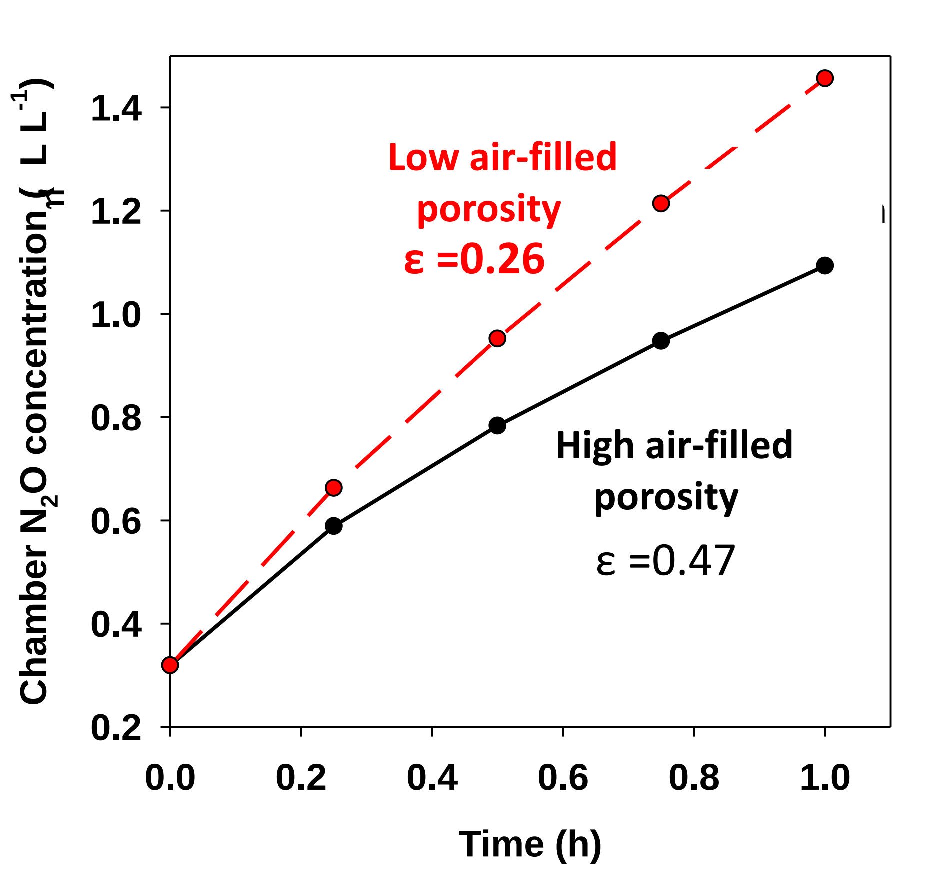


- Bias varies with water content
- Create artifacts & apparent differences

Venterea et al. (2009)

Soil Property Effects on Chamber Dynamics

- Not widely recognized, theory says can be very important
- Modeling: Soil w/ greater ε appears to have lower flux when $Flux_0$ is the same
- After placement, more gas accumulates within soil as opposed to chamber



Venterea & Baker (2008)

Protocol Design Guidance

Chamber height
15 cm

Soil properties
Use <u>minimum expected values</u> of bulk density and water content, e.g.:
1.0 g cm^{-3}
0.10 g g^{-1}

Flux calculation method
Quadratic

Flux-Estimation Error Analysis

Maximum Allowable Deployment time to achieve a given level of bias.

Will set upper limit on bias for the expected "worst-case" soil condition.

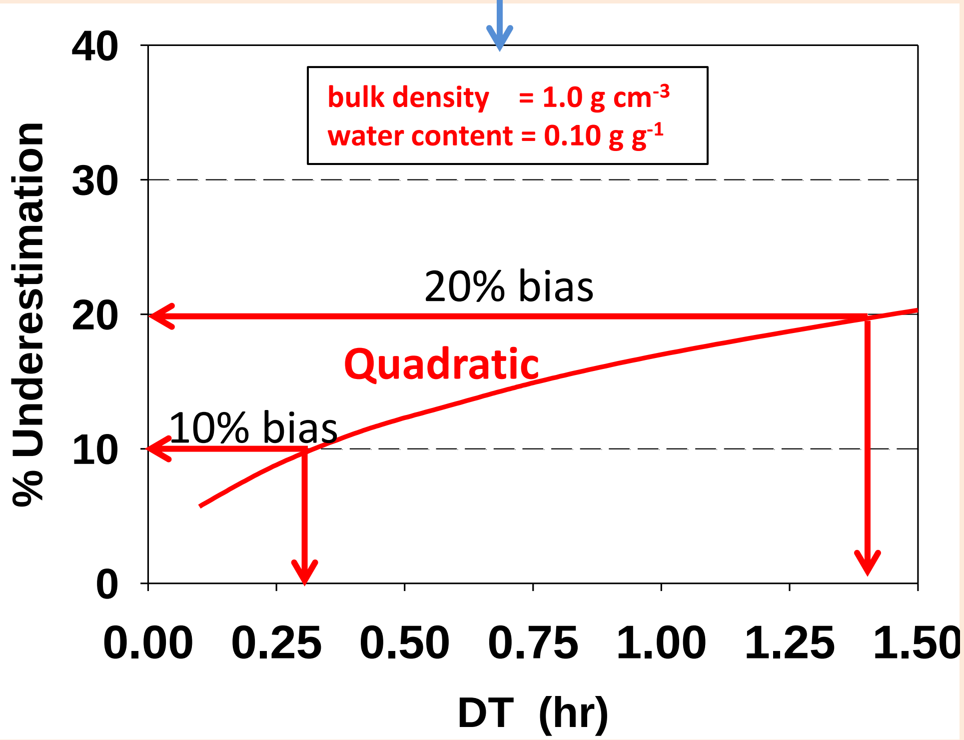
Protocol Design Guidance

Chamber height
15 cm

Soil properties
Use minimum expected values of bulk density and water content, e.g.:
$1.0\ g\ cm^{-3}$
$0.10\ g\ g^{-1}$

Flux calculation method
Quadratic

Flux-Estimation Error Analysis



Protocol Design Guidance

Theoretically-based criteria for establishing protocols that can:

Decrease absolute biases and artifacts arising from differences in soil properties

Problem: Optimum protocols cannot always be used

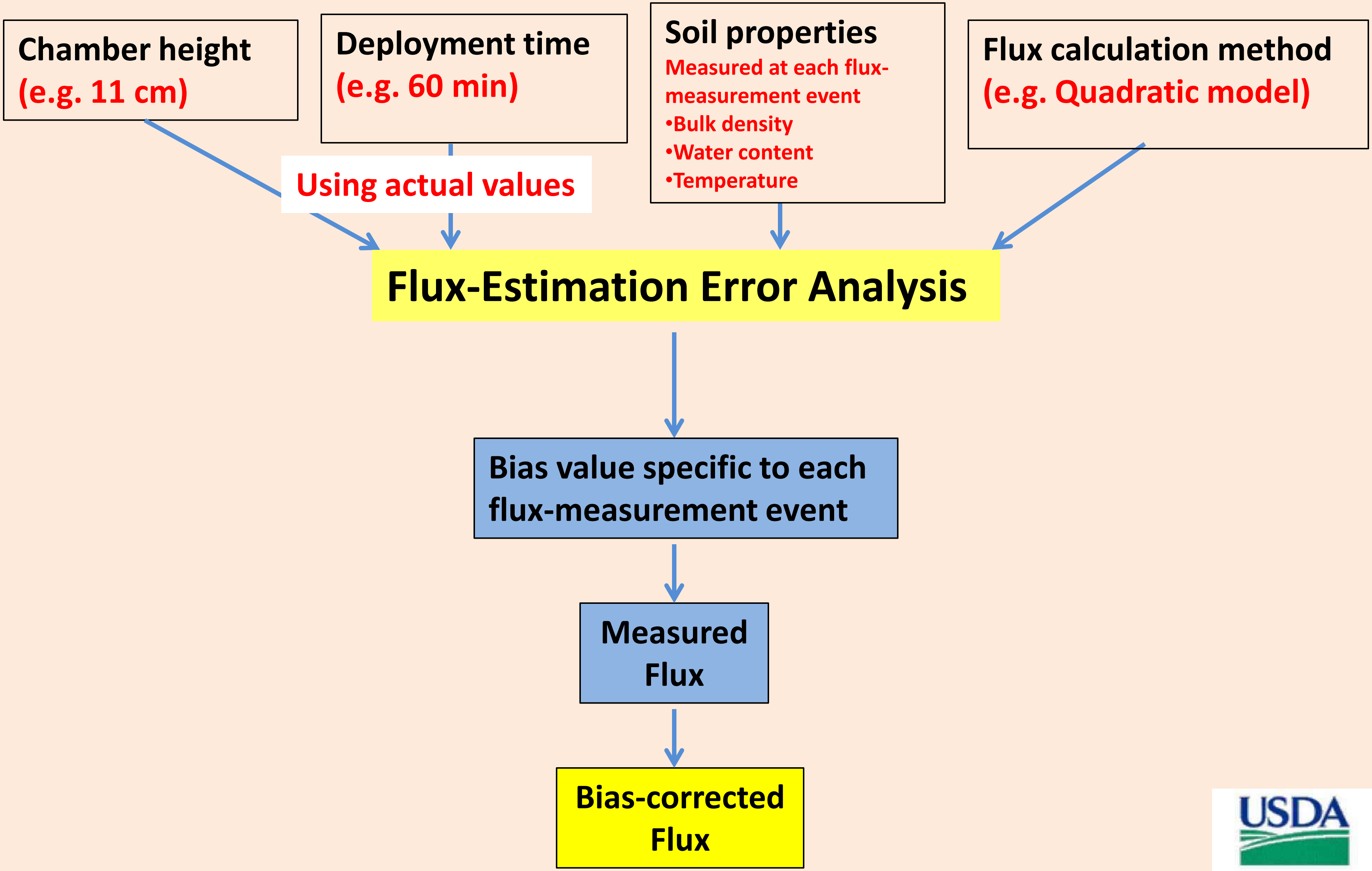
Larger Chamber Heights and Shorter Chamber Deployment Times can be problematic:

1. ***Increased variance due to measurement error***
2. ***Lower sensitivity to detecting fluxes (T. Parkin)***
3. ***Logistical considerations***

   e.g. rotational sampling regimes with large numbers of chamber locations don't allow use of short deployment times

Solutions?

Post-Hoc Bias Correction



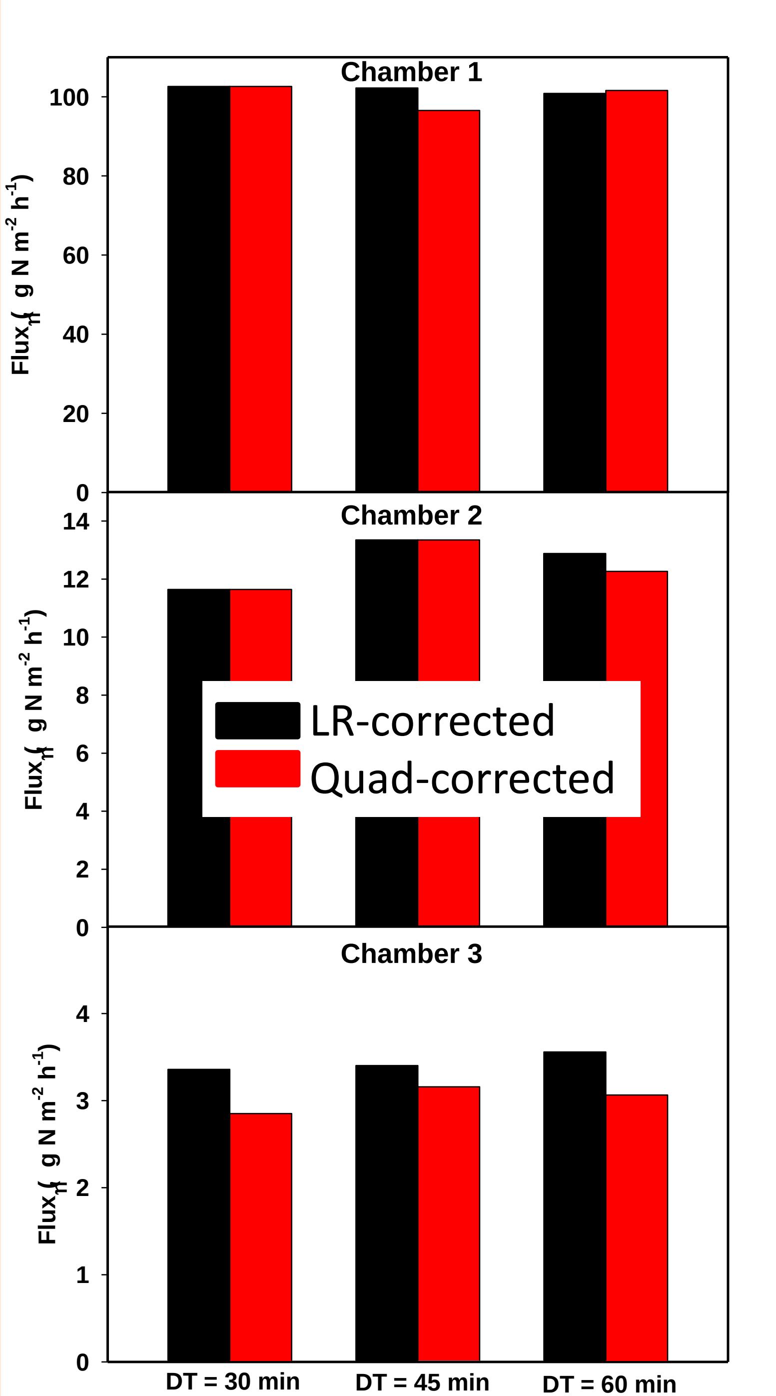
Post-Hoc Bias Correction

Practical Limitations

1. ***Physical Soil Property Measurements*** **required; WFPS & soil temp commonly measured, provide most requirements. Also introduce additional sources of error; more work required to evaluate sensitivity of method to these error sources.**

2. ***Difficult to validate method*****, true** $Flux_0$ **cannot be known under field conditions; laboratory methods might be useful but difficult to simulate field conditions.**

Empirical Evaluation



- Reasonable agreement between bias-corrected flux estimates using:

-Different DTs (30, 45, 60 min)
-Different flux-calculation methods (LR and Quad)

- Some degree of validation, more work needed.

Venterea (2010)

Theoretical Limitations

NDFE model also has simplifying assumptions:

$$S\frac{\partial C}{\partial t} = D_s\frac{\partial^2 C}{\partial z^2} + P(z)$$

1. **Soil is vertically uniform (*S* and D_s are constants)**

Theoretical Limitations

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1. **Soil is vertically uniform (*S* and D_s are constants)**
2. **Transport is limited to 1 D diffusion**
3. **So sink term for N_2O consumption**

Theoretical Limitations

Numerical solutions with non-uniform soil, with lateral diffusion, and sink term allowed:

$$S(z)\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(D_s \frac{\partial C}{\partial z}\right) + \frac{\partial}{\partial y}\left(D_s \frac{\partial C}{\partial y}\right) + P(z) + S(z)$$

Analytical solution reasonably accurate:

1. **When soil physical properties averaged over the upper 10 cm of soil are used as model inputs** *(Venterea and Parkin, 2010)*

2. **Except in highly porous soils (ε > 0.4) and with shallow chamber insertion depths (< 2 cm)** *(unpublished analysis)*

3. **Except when N_2O consumption >> N_2O production** *(Venterea and Stanenas, 2007)*

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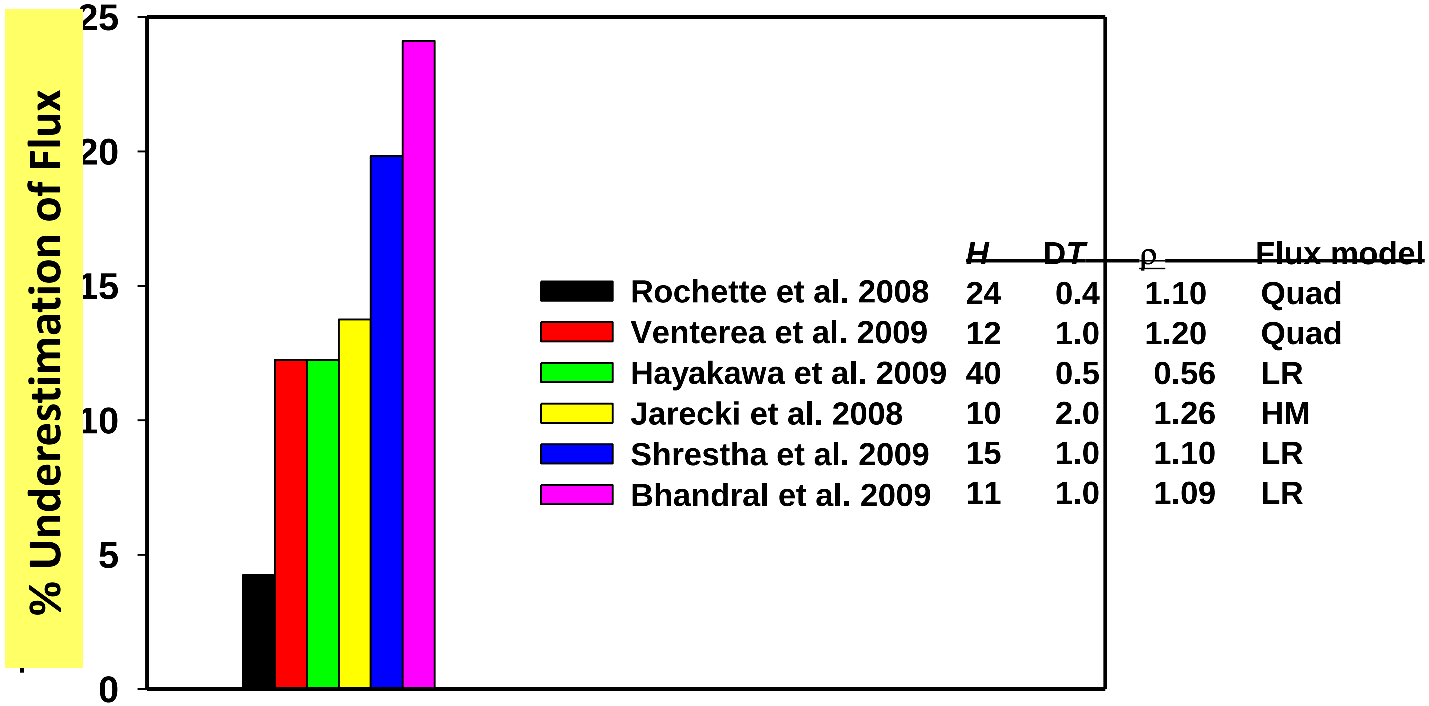
Cross-Study Error Analysis



Assumes water content of 0.25 cm^{-3} cm^{-3}

- **Wide range of measurement conditions, soil properties, and flux-calculation methods leads to a wide range in flux biases across studies.**

- **Raises questions about validity of cross-site comparisons, large-scale emissions estimates and model validation studies; Calls for methods improvements and more uniformity.**

Venterea (2010)

Concluding Remarks

• Bias problems would be largely solved if chamber Deployment Times could be reduced to < 5 or 10 minutes.

• Need high-precision analytical instruments capable of detecting fluxes with short DTs and with minimal measurement error (CV of 1% or less) at ambient concentrations.

• Until these instruments are widely available, methods described here could be useful for decreasing chamber-induced biases.